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Identification of the initial function for discretized delay differential equations

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Abstract

In the present work, we analyze a discrete analogue for the problem of the identification of the initial function for a delay differential equation (DDE) discussed by Baker and Parmuzin in 2004. The basic problem consists of finding an initial function that gives rise to a solution of a discretized DDE, which is a close fit to observed data.

In the continuous problem (finding an initial function that gives rise to a solution of a DDE) studied in 2004 by Baker and Parmuzin, the function is obtained by minimizing a functional $S_\alpha^{\beta,\gamma}(\varphi)$. Here, we use a stepsize h to introduce a discrete version of the problem, along with h-dependent discrete functionals $({}^h\widetilde{S}_\alpha^{\beta,\gamma}(\widetilde{\varphi}))$ that simulate $S_\alpha^{\beta,\gamma}(\varphi)$. Conditions for a minimum of ${}^h\widetilde{S}_\alpha^{\beta,\gamma}(\widetilde{\varphi})$ are explored through an analysis of its first variation ${}^h\widetilde{P}_\alpha^{\beta,\gamma}(\widetilde{\varphi})$, and an iterative technique for obtaining the minimum is written down. In order to explore the properties of this iteration, it is convenient to relate it to an iterative algorithm for the solution of a discretized integral equation (a summation equation), for which the properties of the "kernel" can be obtained. A rôle for adjoint equations and fundamental solutions in the discrete case is established. The final part of the paper consists of a report of numerical experiments that demonstrate the performance of the algorithm.

Keywords: Discrete delay differential equations; Initial function; Discrete adjoint equations; Identification problem; Data assimilation; Discrete fundamental matrices; Regularization parameter

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1. Introduction

Consider an *n*-dimensional system of linear delay differential equations (DDEs) with *time-dependent* coefficients, of the form

$$\frac{\mathrm{d}y(t)}{\mathrm{d}t} - A(t)y(t) - B(t)y(t-\tau) = f(t), \quad \text{for } t \in [0, T], \tag{1a}$$

subject to

$$y(t) = \varphi(t), \quad \text{for } t \in [-\tau, 0]. \tag{1b}$$

Here, τ is a prescribed positive constant (the "lag"), and we suppose

$$y(t),\ f(t),\ \varphi(t) \in \mathbb{R}^{n\times 1}, \quad A(t),\ B(t) \in \mathbb{R}^{n\times n}$$

and these functions will be assumed to be continuous on $[0, T]$. The solution $y(t)$ depends (in particular) upon the initial function $\varphi(t)$; $y(t) \equiv y(\varphi; t)$. The problem that we address is related to the identification of $\varphi(t)$ given τ, $f(t)$, $A(t)$, and $B(t)$, and knowing $y(\varphi; t)$; we shall here study a discrete analogue but we address the continuous problem, briefly, in order to set the scene.

1.1. *The continuous data assimilation problem*

For the continuous identification problem [8,9], we introduced the functional

$$S_\alpha^{\beta,\gamma}(\varphi) := \frac{\alpha}{2}\int_{-\tau}^{0} \|\varphi(t) - \widehat{\varphi}(t)\|^2\,\mathrm{d}t + \frac{\beta}{2}\|\varphi(0) - \widehat{\varphi}(0)\|^2 + \frac{\gamma}{2}\|y(\varphi; 0) - \widehat{y}(0)\|^2 + \frac{1}{2}\int_{0}^{\mathrm{T}} \|y(\varphi; t) - \widehat{y}(t)\|^2\,\mathrm{d}t \tag{2}$$

(in which $\alpha, \beta, \gamma \geqslant 0$ and $y(\varphi; 0) = \varphi(0)$) and $\widehat{\varphi} = \widehat{\varphi}(t)$ and $\widehat{y} = \widehat{y}(t)$ are the given functions and where $y(\varphi; t)$ satisfies (1). The function $\widehat{\varphi}(t)$ contains information about an expected form of $\varphi(t)$. The function $\widehat{y}(t)$ is based on observations of the solution.

The *data assimilation problem* (as the identification problem is called) can be formulated as follows:

Definition 1.1. Let $\mathscr{F} \subseteq \mathscr{PC}\,[-\tau, 0]$ denote a smoothness class of bounded functions on $[-\tau, 0]$. Then the corresponding data assimilation problem for the identification of φ reads as follows:

Define by $y(\varphi; t)$ the solution of (1) with initial function φ. Find $\varphi_\star \in \mathscr{F}$, such $y(\varphi_\star; t)$ minimizes $S_\alpha^{\beta,\gamma}(\varphi)$ over $\mathscr{F}$:

$$\varphi_\star = \arg\min_{\varphi\in\mathscr{F}} S_\alpha^{\beta,\gamma}(\varphi), \tag{3}$$

where $S_\alpha^{\beta,\gamma}(\varphi)$ is defined by (2) in terms of $y(\varphi; t)$.

This formulation embodies parameters $\alpha \geqslant$ and $\beta \geqslant 0$, $\gamma \geqslant 0$, which (when positive) are "regularization parameters" (see [10], for example).

Similar problems have been discussed for ODEs and PDEs, see [1–3,12,15], in particular for the discrete analogue, see [14]. A functional of the type (2) was considered, for example, in [13]. For discussion of related questions for DDEs see [4–6,11,16].

2. A discretized data assimilation problem

In practice, one might endeavour to obtain a discretized version of the data assimilation problem in Definition 1.1 through the use of high-order approximate methods that adapt to any possible discontinuities in the derivatives of the solution $y(\varphi; t)$. It proves rather difficult to analyze such adaptive discretizations in a rigorous manner. We therefore adopt a more limited approach, in order to gain insight.

For a stepsize h with $\tau = Nh$ and $T = Kh$, where N, K are both integers, we introduce $t_n = nh$ ($n \in \{-N, 1-N, \ldots, -1, 0, 1, \ldots, K\}$) and define a *uniform grid* with step size *h*,

$$-\tau = t_{-N} < t_{1-N} < \cdots < t_{-1} < 0 = t_0 < t_1 < \cdots < t_N < t_{N+1} < \cdots < t_K = T.$$

We introduce a discretized equation that results from application of an *Euler formula* to (1). Given the grid above, the explicit Euler equations, for the DDE in (1), read

$$\widetilde{y}_{n+1} - \widetilde{y}_n - hA_n\widetilde{y}_n - hB_n\widetilde{y}_{n-N} = hf_n, \quad \text{for } n \in \{0, 1, \ldots, K-1\}. \tag{4a}$$

Here $\widetilde{y}_n \approx y(\varphi; t_n)$, $B_n = B(nh)$, $A_n = A(nh)$, $f_n = f(nh)$, $\widetilde{\varphi}_n = \varphi(nh)$. The solution is subject to the initial condition

$$\widetilde{y}_n = \widetilde{\varphi}_n, \quad \text{for } -N \leqslant n \leqslant 0 \tag{4b}$$

and it is therefore appropriate to write

$$\widetilde{y}_n = \widetilde{y}_n(\widetilde{\varphi}). \tag{4c}$$

Let us also introduce a discrete analogue of the objective function (2). One possibility is the form

$$\frac{\alpha h}{2}\sum_{n=-N}^{-1}\|\widetilde{\varphi}_n - \widehat{\varphi}(t_n)\|^2 + \frac{h}{2}\sum_{n=0}^{K-1}\|\widetilde{y}_n - \widehat{y}(t_n)\|^2 + \frac{\beta}{2}\|\widetilde{\varphi}_0 - \widehat{\varphi}(t_0)\|^2 + \frac{\gamma}{2}\|\widetilde{y}_0 - \widehat{y}(t_0)\|^2. \tag{5}$$

This discretization is associated with the left-hand (explicit) Euler rule applied to the integrals that define (2), and at this stage it is not transparent that this is a convenient or appropriate discretization.

For flexibility of approach, we generalize (5) by introducing a suitable set of integers $\{p, q, r, s\}$, and the notation

$$\mathfrak{I} := \{p, q, r, s\} \cup \{\alpha, \beta, \gamma\} \tag{6}$$

and write

$$^h\widetilde{S}_{\mathfrak{I}}(\varphi_n) = \frac{\alpha h}{2}\sum_{n=p}^{q}\|\widetilde{\varphi}_n - \widehat{\varphi}(t_n)\|_2^2 + \frac{h}{2}\sum_{n=r}^{s}\|\widetilde{y}_n - \widehat{y}(t_n)\|_2^2 + \frac{\beta}{2}\|\widetilde{\varphi}_0 - \widehat{\varphi}(t_0)\|_2^2 + \frac{\gamma}{2}\|\widetilde{y}_0 - \widehat{y}(t_0)\|_2^2. \tag{7}$$

For example, the expression (5) arises from ${}^h\widetilde{S}_{\mathfrak{J}}(\varphi_n)$ on taking

$$p = -N, \quad q = -1, \quad r = 0, \quad \text{and} \quad s = K - 1. \tag{8}$$

We anticipate the results of our analysis by introducing the notation

$$\begin{aligned} {}^h\widetilde{S}_\alpha^{\beta,\gamma} := {}^h\widetilde{S}_{\mathfrak{J}}(\varphi_n) = \frac{\alpha h}{2} \sum_{n=-N}^{-1} \|\widetilde{\varphi}_n - \widehat{\varphi}(t_n)\|_2^2 + \frac{h}{2} \sum_{n=0}^{K} \|\widetilde{y}_n - \widehat{y}(t_n)\|_2^2 \\ + \frac{\beta}{2} \|\widetilde{\varphi}_0 - \widehat{\varphi}(t_0)\|_2^2 + \frac{\gamma}{2} \|\widetilde{y}_0 - \widehat{y}(t_0)\|_2^2, \end{aligned} \tag{9}$$

which corresponds to the choice $\mathfrak{J}$ in which

$$p = -N, \quad q = -1, \quad r = 0, \quad \text{and} \quad s = K. \tag{10}$$

Prima facie, this is not the most natural choice but will be suggested by the analysis.

For further analysis we shall need to write down a discrete analogue of the adjoint of (1); this we shall regard as an adjoint for (4).

Definition 2.1. (a) Given functions $p^{\mathrm{T}}(t)$ and $\psi^{\mathrm{T}}(t) \in \mathbb{R}^{1\times n}$ (for $t \in [0, T]$ and for $t \in [T, T + \tau]$, respectively, the corresponding *formal adjoint* for (1) is

$$\frac{\mathrm{d}x^{\mathrm{T}}(t)}{\mathrm{d}t} + x^{\mathrm{T}}(t)A(t) + x^{\mathrm{T}}(t+\tau)B(t+\tau) = p^{\mathrm{T}}(t), \quad t \in [0, T], \tag{11a}$$

subject to

$$x^{\mathrm{T}}(t) = \psi^{\mathrm{T}}(t), \quad t \in [T, T + \tau] \tag{11b}$$

with a solution $x^{\mathrm{T}}(t) \in \mathbb{R}^{1\times n}$.

(b) A discrete analogue of the adjoint equation (11) corresponding to (4), is

$$\widetilde{x}_n^{\mathrm{T}} = \widetilde{x}_{n+1}^{\mathrm{T}} + h\widetilde{x}_{n+1}^{\mathrm{T}} A_{n+1} + h\widetilde{x}_{n+N+1}^{\mathrm{T}} B_{n+N+1} + hp_{n+1}^{\mathrm{T}}, \quad n = 0, 1, \ldots, K - 1, \tag{12a}$$

subject to

$$\widetilde{x}_n^{\mathrm{T}} = 0, \quad n = K, \ldots, K + N. \tag{12b}$$

We shall refer to (11a) as a "formal adjoint equation" for (1a) and (12a) as a "formal discrete adjoint equation" for (4).

Remark 2.1. We obtain (12) from (11) by using the backward Euler formula ("backward" for increasing t).

3. The discretized minimization problem

In this section, we formulate a discrete analogue of the problem of identifying an optimal initial function. We are concerned to find the minimum of (7) over the space $\mathscr{F}^h$ of mesh functions defined on points, say $\{t_n\}_{n=-N}^{0} = \{nh\}_{n=-N}^{0}$, where $h = \tau/N$.

In order to find the minimum of ${}^h\widetilde{S}_{\mathfrak{J}}(\widetilde{\varphi})$, we need to find its first variation (compare [8,9]). To write down ${}^h\widetilde{S}_{\mathfrak{J}}(\widetilde{\varphi}+\varepsilon\widetilde{\psi})$ we need an expression for $\widetilde{y}_n(\widetilde{\varphi}+\widetilde{\varepsilon}\psi)$. Let us define

$$L^h\widetilde{y}_n := \frac{\widetilde{y}_{n+1}-\widetilde{y}_n}{h} - A_n\widetilde{y}_n - B_n\widetilde{y}_{n-N}, \quad n=r,r+1,\ldots,s,\ s>r$$

and $M^h\widetilde{y}_n = \widetilde{\varphi}_n$ for $n=r-N,\ldots,r$. Here $A_n=A(nh)$, $B_n=B(nh)$, $\widetilde{\varphi}_n=\varphi(nh)$. By the linearity of L^h and M^h, we obtain the following result.

Lemma 3.1. *With the notation in* (4c),

$$\widetilde{y}_n(\widetilde{\varphi}+\varepsilon\widetilde{\psi}) = \widetilde{y}_n(\widetilde{\varphi}) + \varepsilon\widetilde{z}_n(\widetilde{\psi}), \tag{13}$$

where $\widetilde{z}_n(\widetilde{\psi})$ *satisfies*

$$L^h\widetilde{z}_n = 0 \quad (\textit{for } n=r,r+1,\ldots,s), \quad s>r \quad \textit{and} \tag{14a}$$

$$M^h\widetilde{z}_n = \widetilde{\psi}_n \quad (\textit{for } n=r-N,\ldots,r). \tag{14b}$$

The perturbed objective function ${}^h\widetilde{S}_{\mathfrak{J}}(\widetilde{\varphi}+\varepsilon\widetilde{\psi})$ has the form

$${}^h\widetilde{S}_{\mathfrak{J}}(\widetilde{\varphi}+\varepsilon\widetilde{\psi}) = \frac{\alpha h}{2}\sum_{n=p}^{q}\|\widetilde{\varphi}_n+\varepsilon\widetilde{\psi}_n-\widehat{\varphi}_n\|_2^2 + \frac{h}{2}\sum_{n=r}^{s}\|\widetilde{y}_n+\varepsilon\widetilde{z}_n-\widehat{y}(t_n)\|_2^2 + {}^h\mathfrak{s}'_0, \tag{15a}$$

where

$${}^h\mathfrak{s}'_0 = \frac{\beta}{2}\|\widetilde{\varphi}_0+\varepsilon\widetilde{\psi}_0-\widehat{\varphi}(t_0)\|_2^2 + \frac{\gamma}{2}\|\widetilde{y}_0(\widetilde{\varphi})+\varepsilon\widetilde{z}_0-\widehat{y}(t_0)\|_2^2. \tag{15b}$$

We may write (15) in the form

$${}^h\widetilde{S}_{\mathfrak{J}}(\widetilde{\varphi}+\varepsilon\widetilde{\psi}) = {}^h\widetilde{S}_{\mathfrak{J}}(\widetilde{\varphi}) + \varepsilon\{{}^h\widetilde{P}_{\mathfrak{J}}(\widetilde{\varphi},\widetilde{\psi})\} + \varepsilon^2\{{}^h\widetilde{Q}_{\mathfrak{J}}(\widetilde{\psi})\}, \tag{16}$$

where

$${}^h\widetilde{P}_{\mathfrak{J}}(\widetilde{\varphi},\widetilde{\psi}) = \alpha h\sum_{n=p}^{q}[\widetilde{\varphi}_n-\widehat{\varphi}_n]^{\mathrm{T}}\widetilde{\psi}_n + h\sum_{n=r}^{s}[\widetilde{y}_n-\widehat{y}(t_n)]^{\mathrm{T}}\widetilde{z}_n + {}^h\mathfrak{p}_0 \tag{17a}$$

with

$${}^h\mathfrak{p}_0 = \beta[\widetilde{\varphi}_0-\widehat{\varphi}(t_0)]^{\mathrm{T}}\widetilde{\psi}_0 + \gamma[\widetilde{y}_0(\widetilde{\varphi}_0)-\widehat{y}(t_0)]^{\mathrm{T}}\widetilde{z}_0. \tag{17b}$$

Further,

$${}^h\widetilde{Q}_{\mathfrak{J}}(\widetilde{\psi}) = \frac{\alpha h}{2}\sum_{n=p}^{q}\|\widetilde{\psi}_n\|_2^2 + \frac{h}{2}\sum_{n=r}^{s}\|\widetilde{z}_n\|_2^2 + \frac{\beta}{2}\|\widetilde{\psi}_0\|_2^2 + \frac{\gamma}{2}\|\widetilde{z}_0\|_2^2. \tag{18}$$

Then, we can state the following result.

Theorem 3.1. *A function* $\widetilde{\varphi}$ *defined on* $[-\tau,0]$ *minimizes* ${}^h\widetilde{S}_{\mathfrak{J}}(\widetilde{\varphi})$ *for* $\widetilde{\varphi}\in\mathscr{F}^h$ *if and only if the first variation* ${}^h\widetilde{P}_{\mathfrak{J}}(\widetilde{\varphi},\widetilde{\psi})$ *vanishes for all* $\widetilde{\psi}\in\mathscr{F}^h$, *where* $\widetilde{z}=\widetilde{z}(\widetilde{\psi})$ *satisfies* (14).

3.1. A formula for the first variation

In this section, our objective is to obtain (Lemma 3.2 below) a representation of ${}^h\widetilde{P}_{\mathfrak{J}} \equiv {}^h\widetilde{P}_{\mathfrak{J}}(\widetilde{\varphi}, \widetilde{\psi})$, in terms of the functions $\widetilde{\varphi}$ and $\widetilde{\psi}$. We employ a representation of ${}^h\widetilde{P}_{\mathfrak{J}}$ obtained using a discrete analogue of the adjoint equation. Let us consider (compare (12a))

$$\widetilde{x}_{n-1}^{\mathrm{T}} = \widetilde{x}_n^{\mathrm{T}} + h\widetilde{x}_n^{\mathrm{T}} A_n + h\widetilde{x}_{n+N}^{\mathrm{T}} B_{n+N} + h[\widetilde{y}_n(\widetilde{\varphi}) - \widehat{y}_n]^{\mathrm{T}}, \quad n = r, \ldots, s \tag{19a}$$

with

$$\widetilde{x}_n^{\mathrm{T}} = 0, \quad n = s, \ldots, s + N. \tag{19b}$$

(If, for example, $r = 0$, (19a) defines a value $\widetilde{x}_{-1}$.)

For appropriate r and s this is a discrete version of the adjoint equation appearing in [8, p. 4, 9], discretized using the implicit Euler formula. We can write (17a) in the form

$$\begin{aligned}
{}^h\widetilde{P}_{\mathfrak{J}} &= \beta[\widetilde{\varphi}_0 - \widehat{\varphi}(t_0)]^{\mathrm{T}}\widetilde{\psi}_0 + \gamma[\widetilde{y}_0(\widetilde{\varphi}_0) - \widehat{y}(t_0)]^{\mathrm{T}}\widetilde{z}_0 \\
&\quad + \alpha h \sum_{n=p}^{q} [\widetilde{\varphi}_n - \widehat{\varphi}_n]^{\mathrm{T}}\widetilde{\psi}_n + \sum_{n=r}^{s} \left(\underbrace{(\widetilde{x}_{n-1}^{\mathrm{T}} - \widetilde{x}_n^{\mathrm{T}})\widetilde{z}_n}_{\mathscr{J}_1} - h\widetilde{x}_n^{\mathrm{T}} A_n \widetilde{z}_n - \underbrace{h\widetilde{x}_{n+N}^{\mathrm{T}} B_{n+N}\widetilde{z}_n}_{\mathscr{J}_2} \right).
\end{aligned}$$

- Using summation by parts we can write $\mathscr{J}_1$ as

$$\mathscr{J}_1 \equiv \sum_{n=r}^{s} (\widetilde{x}_{n-1}^{\mathrm{T}} - \widetilde{x}_n^{\mathrm{T}})\widetilde{z}_n = -\widetilde{x}_s^{\mathrm{T}}\widetilde{z}_{s+1} + \widetilde{x}_{r-1}^{\mathrm{T}}\widetilde{z}_r + \sum_{n=r}^{s} \widetilde{x}_n^{\mathrm{T}}(\widetilde{z}_{n+1} - \widetilde{z}_n).$$

- For the term $\mathscr{J}_2$ we have

$$\begin{aligned}
\mathscr{J}_2 &\equiv h \sum_{n=r}^{s} \widetilde{x}_{n+N}^{\mathrm{T}} B_{n+N}\widetilde{z}_n \\
&= h \sum_{n=r}^{s} \widetilde{x}_n^{\mathrm{T}} B_n \widetilde{z}_{n-N} - \underbrace{h \sum_{n=r}^{r+N-1} \widetilde{x}_n^{\mathrm{T}} B_n \widetilde{z}_{n-N}}_{\mathscr{J}_3} + h \sum_{n=s+1}^{s+N} \widetilde{x}_n^{\mathrm{T}} B_n \widetilde{z}_{n-N}.
\end{aligned}$$

We can write the term $\mathscr{J}_3$ in the form $\mathscr{J}_3 = h\sum_{n=r}^{r+N-1} \widetilde{x}_n^{\mathrm{T}} B_n \widetilde{z}_{n-N} = h\sum_{n=r-N}^{r-1} \widetilde{x}_{n+N}^{\mathrm{T}} B_{n+N}\widetilde{z}_n$. Therefore, (17a) has the form

$$\begin{aligned}
{}^h\widetilde{P}_{\mathfrak{J}} &= {}^h\mathfrak{p}_0 + h \sum_{n=p}^{q} [\alpha(\widetilde{\varphi}_n - \widehat{\varphi}_n)]^{\mathrm{T}}\widetilde{\psi}_n + h \sum_{n=r-N}^{r-1} \widetilde{x}_{n+N}^{\mathrm{T}} B_{n+N}\widetilde{z}_n + \widetilde{x}_{r-1}^{\mathrm{T}}\widetilde{z}_r - \widetilde{x}_s^{\mathrm{T}}\widetilde{z}_{s+1} \\
&\quad + \sum_{n=r}^{s} \widetilde{x}_n^{\mathrm{T}}(\widetilde{z}_{n+1} - \widetilde{z}_n - hA_n\widetilde{z}_n - hB_n\widetilde{z}_{n-N}) - h \sum_{n=s+1}^{s+N} \widetilde{x}_n^{\mathrm{T}} B_n \widetilde{z}_{n-N}.
\end{aligned}$$

Let $\widetilde{z}_n$ satisfy $\widetilde{z}_{n+1} - \widetilde{z}_n - hA_n\widetilde{z}_n - hB_n\widetilde{z}_{n-N} = 0$, for $n = r, r+1, \ldots, s$, with $\widetilde{z}_n = \widetilde{\psi}_n$, $n = r-N, \ldots, r$. (Compare [8, pp. 7–8, 9].) Taking into account (19), we obtain

$$ {}^h\widetilde{P}_{\mathfrak{I}} = {}^h\mathfrak{p}_0 + h\sum_{n=p}^{q} [\alpha(\widetilde{\varphi}_n - \widehat{\varphi}_n)]^{\mathrm{T}}\widetilde{\psi}_n + h\sum_{n=r-N}^{r-1} \widetilde{x}^{\mathrm{T}}_{n+N}B_{n+N}\widetilde{\psi}_n + \widetilde{x}^{\mathrm{T}}_{r-1}\widetilde{\psi}_r, $$

which is independent of our choice of s.

Now, from (19), $\widetilde{x}^{\mathrm{T}}_{r-1} = \widetilde{x}^{\mathrm{T}}_r + h\widetilde{x}^{\mathrm{T}}_r A_r + h\widetilde{x}^{\mathrm{T}}_{r+N}B_{r+N} + h[\widetilde{y}_r(\widetilde{\varphi}_n) - \widehat{y}_r]^{\mathrm{T}}$. Therefore,

$$ \begin{aligned} {}^h\widetilde{P}_{\mathfrak{I}} = {}^h\mathfrak{p}_0 &+ h\sum_{n=p}^{q} \alpha(\widetilde{\varphi}_n - \widehat{\varphi}_n)^{\mathrm{T}}\widetilde{\psi}_n + h\sum_{n=r-N}^{r-1} \widetilde{x}^{\mathrm{T}}_{n+N}B_{n+N}\widetilde{\psi}_n \\ &+ (\widetilde{x}^{\mathrm{T}}_r(1 + hA_r) + h\widetilde{x}^{\mathrm{T}}_{r+N}B_{r+N} + h[\widetilde{y}_r(\widetilde{\varphi}_n) - \widehat{y}_r]^{\mathrm{T}})\widetilde{\psi}_r. \end{aligned} $$

We now set (leave s undefined), as in (8),

$$ p = r - N, \quad q = r - 1 \tag{20} $$

and, since the term ${}^h\mathfrak{p}_0$ depends on function values at $t = 0$ it is convenient to set $r = 0$. Then, we have

$$ \begin{aligned} {}^h\widetilde{P}_{\mathfrak{I}} = h\sum_{n=-N}^{-1} &([\alpha(\widetilde{\varphi}_n - \widehat{\varphi}_n)]^{\mathrm{T}} + \widetilde{x}^{\mathrm{T}}_{n+N}B_{n+N})\widetilde{\psi}_n + (\beta[\widetilde{\varphi}_0 - \widehat{\varphi}(t_0)]^{\mathrm{T}} + \gamma[\widetilde{y}_0(\widetilde{\varphi}_n) - \widehat{y}(t_0)]^{\mathrm{T}} \\ &+ \widetilde{x}^{\mathrm{T}}_0(1 + hA_0) + h\widetilde{x}^{\mathrm{T}}_N B_N + h[\widetilde{y}_0(\widetilde{\varphi}) - \widehat{y}_0]^{\mathrm{T}})\widetilde{\psi}_0. \end{aligned} \tag{21} $$

The first variation must be zero for all $\widetilde{\psi}$ in $\mathscr{F}^h$, therefore we obtain the following result.

Lemma 3.2. *A function $\widetilde{\varphi}^\star$ defined on $[-\tau, 0]$ which minimizes ${}^h\widetilde{S}_{\mathfrak{I}}(\widetilde{\varphi})$ for $\widetilde{\varphi} \in \mathscr{F}^h$ satisfies the equations*

$$ \alpha(\widetilde{\varphi}^\star_n - \widehat{\varphi}_n) + [\widetilde{x}^{\mathrm{T}}_{n+N}B_{n+N}]^{\mathrm{T}} = 0, \quad n = -N, \ldots, -1, \tag{22a} $$

$$ \widetilde{x}^{\mathrm{T}}_0(1 + hA_0) + h\widetilde{x}^{\mathrm{T}}_N B_N + \beta[\widetilde{\varphi}_0 - \widehat{\varphi}(t_0)]^{\mathrm{T}} + (\gamma + h)[\widetilde{y}_0 - \widehat{y}(t_0)]^{\mathrm{T}} = 0, \quad n = 0. \tag{22b} $$

4. A discrete integral equation (or summation equation)

In this section we derive a discrete integral equation (a "summation[1] equation") for the initial function that minimizes ${}^h\widetilde{S}_{\mathfrak{I}}$ (with choice of $\mathfrak{I}$ in which $p = -N$, $q = -1$, $r = 0$ and $s = K$). The equivalence allows us to analyze the properties of the iterative algorithm.

According to Section 3 we should introduce a method for determining the optimal initial function. In Sections 4.1 and 4.2 we retain a general s, but the objective function has the natural form when we set

$$ s = K \tag{23} $$

[1] The summation equation is an analogue of the integral equation obtained in the continuous case in [8, pp. 16–18, 9].

in (6). Following the discussion in Section 3.1 and from the result of Lemma 3.2 we can consider the system of equations of finding the initial function $\widetilde{\varphi}$, which minimizes ${}^h\widetilde{S}_{\mathfrak{J}}$. We have, for $s = K$,

$$\frac{\widetilde{y}_{n+1} - \widetilde{y}_n}{h} - A_n \widetilde{y}_n - B_n \widetilde{y}_{n-N} = f_n, \quad n = 0, 1, \ldots, K-1, \tag{24a}$$

$$\widetilde{y}_n = \widetilde{\varphi}_n, \quad n = -N, \ldots, 0, \tag{24b}$$

$$-\frac{\widetilde{x}_n^{\mathrm{T}} - \widetilde{x}_{n-1}^{\mathrm{T}}}{h} - \widetilde{x}_n^{\mathrm{T}} A_n - \widetilde{x}_{n+N}^{\mathrm{T}} B_{n+N} = h[\widetilde{y}_n(\widetilde{\varphi}) - \widehat{y}_n]^{\mathrm{T}}, \tag{24c}$$

$$\widetilde{x}_n^{\mathrm{T}} = 0, \quad n = K, \ldots, K+N, \tag{24d}$$

$$\alpha(\widetilde{\varphi}_n - \widehat{\varphi}_n) + B_{n+N}^{\mathrm{T}} \widetilde{x}_{n+N} = 0, \quad n = -N, \ldots, -1, \tag{24e}$$

$$[I + hA_0]^{\mathrm{T}} \widetilde{x}_0 + hB_N^{\mathrm{T}} \widetilde{x}_N + h[\widetilde{y}_0(\widetilde{\varphi}) - \widehat{y}_0] + {}^h\mathfrak{p}_0 = 0. \tag{24f}$$

In the next section we shall establish a discrete integral equation (or "summation equation") for the optimal initial function using formulae for solutions of Eqs. (24a) and (24c), and the additional Eqs. (24e) and (24f) for the initial function.

4.1. *The discrete integral equation in terms of fundamental matrices*

Let us consider the discrete version of the adjoint equation (24c). According to [7, pp. 14–15], we may write the solution of the adjoint equation (24c) in the form

$$\widetilde{x}_k^{\mathrm{T}} = h \sum_{m=k+1}^{s} [\widetilde{y}_m - \widehat{y}_m]^{\mathrm{T}} \widetilde{Y}(m,k),$$

where

$$\widetilde{y}_m = \widetilde{Y}(m,0)\{I + hA_0\}\widetilde{\varphi}_0 + h \sum_{l=-N}^{0} \widetilde{Y}(m, l+N) B_{l+N} \widetilde{\varphi}_l + h \sum_{l=0}^{m-1} \widetilde{Y}(m,l) f_l.$$

(This is a solution of the discrete DDE written in terms of fundamental matrices, see [7, pp. 13–14].) Thus, we can write

$$\widetilde{x}_k^{\mathrm{T}} = h \sum_{m=k+1}^{s} \left[\widetilde{Y}(m,0)\{I + hA_0\}\widetilde{\varphi}_0 + h \sum_{l=-N}^{0} \widetilde{Y}(m, l+N) B_{l+N} \widetilde{\varphi}_l + h \sum_{l=0}^{m-1} \widetilde{Y}(m,l) f_l \right]^{\mathrm{T}}$$
$$\times \widetilde{Y}(m,k) - h \sum_{m=k+1}^{s} [\widehat{y}_m]^{\mathrm{T}} \widetilde{Y}(m,k). \tag{25}$$

We can write for $\widetilde{\varphi}_0$ from (24f)

$$(\beta + \gamma + h) I \widetilde{\varphi}_0 + hB_N^{\mathrm{T}} \widetilde{x}_N + [I + hA_0]^{\mathrm{T}} \widetilde{x}_0 = (\alpha h + \beta)\widehat{\varphi}_0 + (\gamma + h)\widehat{y}_0. \tag{26}$$

Let us define

$$\widetilde{M}_A(m,0) = \widetilde{Y}(m,0)[I + hA_0] \quad \text{and} \quad \widetilde{M}_B(m,N) = h\widetilde{Y}(m,N)B_N. \tag{27}$$

Using the expression for $\widetilde{x}_0^{\mathrm{T}}$ and $\widetilde{x}_N^{\mathrm{T}}$ defined by (25) and taking into account that $\widetilde{Y}(m,N)=0$ when $m\leqslant N$, we can write (26) in the form

$$ {}^h\mathscr{D}^{\beta,\gamma}\widetilde{\varphi}_0 + h\sum_{m=1}^{s}\sum_{l=-N}^{-1}(\widetilde{M}_A^{\mathrm{T}}(m,0)+\widetilde{M}_B^{\mathrm{T}}(m,N))\widetilde{M}_B(m,l+N)\widetilde{\varphi}_l = \mathfrak{f}^{\beta,\gamma}, \tag{28} $$

where $\mathfrak{f}^{\beta,\gamma}=\mathfrak{f}^{\beta,\gamma}(\widehat{\varphi},\widehat{\varphi}_0,\widehat{y},f)$,

$$ {}^h\mathscr{D}^{\beta,\gamma} \equiv (\beta+\gamma+h)I + h\sum_{m=1}^{s}(\widetilde{M}_A^{\mathrm{T}}(m,0)+\widetilde{M}_B^{\mathrm{T}}(m,N))(\widetilde{M}_A(m,0)+\widetilde{M}_B(m,N)) $$

and

$$ \mathfrak{f}^{\beta,\gamma} = \beta I\widehat{\varphi}_0 + (\gamma+h)I\widehat{y}_0 - h\sum_{m=1}^{s}(\widetilde{M}_A^{\mathrm{T}}(m,0)+\widetilde{M}_B^{\mathrm{T}}(m,N))\left(h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l - \widehat{y}_m\right). $$

According to (24e), $\widetilde{\varphi}_n$ satisfies the discrete equation

$$ \alpha\widetilde{\varphi}_n + [\widetilde{x}_{n+N}^{\mathrm{T}}B_{n+N}]^{\mathrm{T}} = \alpha\widehat{\varphi}_n \quad (\text{for } n=-N,\ldots,-1). \tag{29} $$

Thus, by substituting the expression for $\widetilde{x}_{n+N}^{\mathrm{T}}$ from (25) into (29) we obtain a “discrete integral equation” for $\widetilde{\varphi}_n$. Thus, we can state the following results:

Theorem 4.1. *A function $\widetilde{\varphi}$, which minimizes ${}^h\widetilde{S}_\alpha^{\beta,\gamma}(\widetilde{\varphi})$ for $\widetilde{\varphi}\in\mathscr{F}^h$ satisfies the summation equation*

$$ \alpha\widetilde{\varphi}_n + \sum_{l=-N}^{-1}{}^h\mathscr{K}_{nl}^{\beta,\gamma}\widetilde{\varphi}_l = {}^h\mathfrak{g}_\alpha^{\beta,\gamma}(n) \quad \textit{for } n=-N,-1 \tag{30} $$

and

$$ \widetilde{\varphi}_0 = -[{}^h\mathscr{D}^{\beta,\gamma}]^{-1}h\sum_{m=1}^{s}\sum_{l=-N}^{-1}(\widetilde{M}_A^{\mathrm{T}}(m,0)+\widetilde{M}_B^{\mathrm{T}}(m,N))\widetilde{M}_B(m,l+N)\widetilde{\varphi}_l + [{}^h\mathscr{D}^{\beta,\gamma}]^{-1}\mathfrak{f}^{\beta,\gamma}. $$

Here, $\mathfrak{f}^{\beta,\gamma}=\mathfrak{f}^{\beta,\gamma}(\widehat{\varphi},\widehat{\varphi}_0,\widehat{y},f)$, and

$$ \begin{aligned} {}^h\mathscr{K}_{nl}^{\beta,\gamma} &= \sum_{m=1}^{s}\widetilde{M}_B^{\mathrm{T}}(m,n+N)\widetilde{M}_B(m,l+N) \\ &\quad - h\sum_{m=1}^{s}\sum_{j=1}^{s}\mathscr{M}^{\mathrm{T}}(m,n+N)[{}^h\mathscr{D}^{\beta,\gamma}]^{-1}\mathscr{M}(j,l+N), \end{aligned} $$

$$ \begin{aligned} {}^h\mathfrak{g}_\alpha^{\beta,\gamma}(n) &= \alpha\widehat{\varphi}_n - h\sum_{m=1}^{s}\left\{\widetilde{M}_B^{\mathrm{T}}(m,n+N)\left(h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l - \widehat{y}_m\right)\right. \\ &\qquad \left. - \mathscr{M}^{\mathrm{T}}(m,n+N)[{}^h\mathscr{D}^{\beta,\gamma}]^{-1}\mathfrak{f}^{\beta,\gamma}\right\}, \end{aligned} $$

$$\mathscr{M}(m, n+N) = (\widetilde{M}_A^{\mathrm{T}}(m,0) + \widetilde{M}_B^{\mathrm{T}}(m,N))\widetilde{M}_B(m, l+N);$$

$$^h\mathscr{D}^{\beta,\gamma} \equiv (\beta+\gamma+h)I + h\sum_{m=1}^{s}(\widetilde{M}_A^{\mathrm{T}}(m,0) + \widetilde{M}_B^{\mathrm{T}}(m,N))(\widetilde{M}_A(m,0) + \widetilde{M}_B(m,N)), \tag{31}$$

$$\mathfrak{f}^{\beta,\gamma} = \beta I\widehat{\varphi}_0 + (\gamma+h)I\widehat{y}_0 - h\sum_{m=1}^{s}(\widetilde{M}_A^{\mathrm{T}}(m,0) + \widetilde{M}_B^{\mathrm{T}}(m,N))\left(h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l - \widehat{y}_m\right).$$

4.2. Properties of the 'discrete kernel'

We can establish the properties of the 'discrete kernel' by adapting the discussion for the continuous case [8,9]. Let us consider the first variation of the functional (7) with the set of limits (10). We have the general results (16)–(17), and we use the notation

$$^h\widetilde{S}_\alpha^{\beta,\gamma} = {}^h\widetilde{S}_{\mathfrak{J}}(\widetilde{\varphi}), \quad {}^h\widetilde{P}_\alpha^{\beta,\gamma} = {}^h\widetilde{P}_{\mathfrak{J}}(\widetilde{\varphi},\widetilde{\psi}) \quad \text{when } p = -N,\ q = -1,\ r = 0, \text{ and } s = K. \tag{32}$$

Here, $^h\widetilde{S}_\alpha^{\beta,\gamma} = {}^h\widetilde{S}_\alpha^{\beta,\gamma}(\widetilde{\varphi})$, $^h\widetilde{P}_\alpha^{\beta,\gamma} = {}^h\widetilde{P}_\alpha^{\beta,\gamma}(\widetilde{\varphi},\widetilde{\psi})$, etc. Taking into account (21), we can write

$$^h\widetilde{P}_\alpha^{\beta,\gamma} = \alpha h\sum_{n=-N}^{-1}(\widetilde{\varphi}_n - \widehat{\varphi}_n)^{\mathrm{T}}\widetilde{\psi}_n + h\sum_{n=1}^{s}[\widetilde{y}_n(\widetilde{\varphi}) - \widehat{y}_n]^{\mathrm{T}}\widetilde{z}_n + \widehat{\mathfrak{p}}_{\beta,\gamma}^h, \tag{33}$$

where $\widehat{\mathfrak{p}}_{\beta,\gamma}^h$ can be expressed as $^1\widehat{\mathfrak{p}}_{\beta,\gamma}^h(\widetilde{\varphi}_0,\widetilde{\psi}_0) + {}^2\widehat{\mathfrak{p}}_{\beta,\gamma}^h(\widehat{\varphi}_0,\widehat{y}_0,\widetilde{\psi}_0)$ (if we replace the term $[\widetilde{y}_0(\widetilde{\varphi}) - \widehat{y}_0]^{\mathrm{T}}\widetilde{z}_0$ by the term $^2\hat{\mathfrak{p}}_{\beta,\gamma}^h$). We can then write (33)in the form

$$^h\widetilde{P}_\alpha^{\beta,\gamma} = \alpha h\sum_{n=-N}^{-1}\widetilde{\varphi}_n^{\mathrm{T}}\widetilde{\psi}_n - \alpha h\sum_{n=-N}^{-1}\widehat{\varphi}_n^{\mathrm{T}}\widetilde{\psi}_n + h\sum_{n=1}^{s}\widetilde{y}_n^{\mathrm{T}}(\widetilde{\varphi})\widetilde{z}_n - h\sum_{n=1}^{s}\widehat{y}_n^{\mathrm{T}}\widetilde{z}_n + \widehat{\mathfrak{p}}_{\beta,\gamma}^h,$$

or, with an obvious notation,

$$^h\widetilde{P}_\alpha^{\beta,\gamma} = \varDelta_1^h\widetilde{P}_\alpha^{0,0}(\widetilde{\varphi},\widetilde{\psi}) - \varDelta_2^h\widetilde{P}_\alpha^{0,0}(\widehat{\varphi},\widetilde{\psi}) + \nabla_1^h\widetilde{P}_0^{0,0}(\widetilde{y},\widetilde{z}) - \nabla_2^h\widetilde{P}_0^{0,0}(\widehat{y},\widetilde{z}) + \widehat{\mathfrak{p}}_{\beta,\gamma}^h. \tag{34}$$

Using the discrete fundamental solution [7, pp. 13–14], and (27), we have

$$\widetilde{y}_n = \widetilde{M}_A(n,0)\widetilde{\varphi}_0 + h\sum_{l=-N}^{0}\widetilde{M}_B(n,l+N)\widetilde{\varphi}_l + h\sum_{l=0}^{n-1}\widetilde{Y}(n,l)f_l, \tag{35}$$

$$\widetilde{z}_n = \widetilde{M}_A(n,0)\widetilde{\psi}_0 + h\sum_{l=-N}^{0}\widetilde{M}_B(n,l+N)\widetilde{\psi}_l. \tag{36}$$

Thus, using (35) and (36) we can write

$$\begin{aligned}
&\nabla_1^h \widetilde{P}_0^{0,0}(\widetilde{y},\widetilde{z})\\
&\quad = h\sum_{n=1}^{s}\Bigg\{\widetilde{\varphi}_0^{\mathrm{T}}\widetilde{M}_A^{\mathrm{T}}(n,0)\widetilde{M}_A(n,0)\widetilde{\psi}_0 + \sum_{l=-N}^{0}\sum_{m=-N}^{0}\widetilde{\varphi}_l^{\mathrm{T}}\widetilde{M}_B^{\mathrm{T}}(n,l+N)\widetilde{M}_B(n,m+N)\widetilde{\psi}_m\\
&\qquad + h\sum_{l=-N}^{0}\widetilde{\varphi}_0^{\mathrm{T}}\widetilde{M}_A^{\mathrm{T}}(n,0)\widetilde{M}_B(n,l+N)\widetilde{\psi}_l + h\sum_{l=-N}^{0}\widetilde{\varphi}_l^{\mathrm{T}}\widetilde{M}_B^{\mathrm{T}}(n,l+N)\widetilde{M}_A(n,0)\widetilde{\psi}_0\Bigg\}\\
&\qquad + h^2\sum_{n=1}^{s}\sum_{l=0}^{n-1}\widetilde{Y}^{\mathrm{T}}(n,l)f_l^{\mathrm{T}}\left\{\widetilde{M}_A(n,0)\widetilde{\psi}_0 + \sum_{m=-N}^{0}\widetilde{M}_B^{\mathrm{T}}(n,m+N)\widetilde{\psi}_l\right\},
\end{aligned}$$

or, in brief,

$$\nabla_1^h \widetilde{P}_0^{0,0}(\widetilde{y},\widetilde{z}) = {}^1\nabla_1^h \widetilde{P}_0^{0,0}(\widetilde{\varphi},\widetilde{\psi}) + {}^2\nabla_1^h \widetilde{P}_0^{0,0}(f,\widetilde{\psi}).$$

Define

$${}^h\widehat{\mathfrak{P}}_\alpha^{\beta,\gamma}(\widetilde{\varphi},\widetilde{\psi}) = \varDelta_1^h \widetilde{P}_\alpha^{0,0}(\widetilde{\varphi},\widetilde{\psi}) + {}^1\nabla_1^h \widetilde{P}_0^{0,0}(\widetilde{\varphi},\widetilde{\psi}) + {}^1\widehat{\mathfrak{p}}_{\beta,\gamma}^h(\widetilde{\varphi}_0,\widetilde{\psi}_0). \tag{37}$$

Since the equation ${}^h\widetilde{P}_\alpha^{\beta,\gamma} = 0$ reads ${}^h\widetilde{\mathfrak{P}}_\alpha^{\beta,\gamma}(\widetilde{\varphi},\widetilde{\psi}) - (\mathfrak{g},\widetilde{\psi}) = 0$ for appropriate $\mathfrak{g}$ (actually, $\mathfrak{g} = {}^h\mathfrak{g}_\alpha^{\beta,\gamma}$) we now consider the discrete bilinear form (37).

Lemma 4.1. *The discrete bilinear form* ${}^h\widetilde{\mathfrak{P}}_\alpha^{\beta,\gamma}(\widetilde{\varphi},\widetilde{\psi})$ *in* (37) *is symmetric, and positive definite* $({}^h\widetilde{\mathfrak{P}}_\alpha^{\beta,\gamma}(\widetilde{\varphi},\widetilde{\varphi}) > 0$ *if* $\{\widetilde{\varphi}_n\} \neq 0)$ *on* $\mathscr{F}^h$ *for* $\alpha \geqslant 0$.

Proof. Let us write the term ${}^1\nabla_1^h \widetilde{P}_0^{0,0}(\widetilde{\varphi},\widetilde{\psi})$ in the form

$$h\sum_{n=1}^{s}\left[\widetilde{M}_A(n,0)\widetilde{\varphi}_0 + \sum_{l=-N}^{0}\widetilde{M}_B(n,l+N)\widetilde{\varphi}_l\right]^{\mathrm{T}}\left[\widetilde{M}_A(n,0)\widetilde{\psi}_0 + \sum_{l=-N}^{0}\widetilde{M}_B(n,l+N)\widetilde{\psi}_l\right],$$

where ${}^1\widehat{\mathfrak{p}}_{\beta,\gamma}^h(\widetilde{\varphi}_0,\widetilde{\psi}_0) = (\beta+\gamma+h)\widetilde{\varphi}_0^{\mathrm{T}}\widetilde{\psi}_0$. Thus, for ${}^h\widetilde{\mathfrak{P}}_\alpha^{\beta,\gamma}(\widetilde{\varphi},\widetilde{\psi})$ we have

$$\begin{aligned}
{}^h\mathfrak{P}_\alpha^{\beta,\gamma}(\widetilde{\varphi},\widetilde{\psi}) = \alpha h\sum_{n=-N}^{-1}\widetilde{\varphi}_n^{\mathrm{T}}\widetilde{\psi}_n + h\sum_{n=1}^{s}\left[\widetilde{M}_A(n,0)\widetilde{\varphi}_0 + \sum_{l=-N}^{0}\widetilde{M}_B(n,l+N)\widetilde{\varphi}_l\right]^{\mathrm{T}}&\\
\times\left[\widetilde{M}_A(n,0)\widetilde{\psi}_0 + \sum_{l=-N}^{0}\widetilde{M}_B(n,l+N)\widetilde{\psi}_l\right] + (\beta+\gamma+h)\widetilde{\varphi}_0^{\mathrm{T}}\widetilde{\psi}_0&
\end{aligned}\tag{38}$$

and it is straightforward from (38) that ${}^h\widetilde{\mathfrak{P}}_\alpha^{\beta,\gamma}(\widetilde{\varphi},\widetilde{\psi})$ is symmetric and ${}^h\widetilde{\mathfrak{P}}_\alpha^{\beta,\gamma}(\widetilde{\varphi},\widetilde{\varphi}) > 0$. With $\alpha = 0$ the quadratic form $({}^h\widetilde{\mathfrak{P}}_0^{\beta,\gamma}(\widetilde{\varphi},\widetilde{\varphi}))$ remains symmetric and positive definite. The Lemma is therefore established. $\square$

We shall now obtain a result concerning ${}^{h}\mathscr{K}^{\beta,\gamma}_{lm}$ in Theorem 4.1. Collecting the similar terms in (38) we obtain

$$
\begin{aligned}
{}^{h}\widetilde{\mathfrak{P}}^{\beta,\gamma}_{\alpha}(\widetilde{\varphi},\widetilde{\psi}) = {}& h\sum_{n=1}^{s}\sum_{l=-N}^{-1}\sum_{m=-N}^{-1}\widetilde{\varphi}_l^{\mathrm{T}}\widetilde{M}_B^{\mathrm{T}}(n,l+N)\widetilde{M}_B(n,m+N)\widetilde{\psi}_m + \alpha h\sum_{l=-N}^{-1}\widetilde{\varphi}_l^{\mathrm{T}}\widetilde{\psi}_l \\
& + h\sum_{n=1}^{s}\sum_{l=-N}^{-1}\widetilde{\varphi}_l^{\mathrm{T}}\widetilde{M}_B^{\mathrm{T}}(n,l+N)[\widetilde{M}_A(n,0)+\widetilde{M}_B(n,N)]\widetilde{\psi}_0 \\
& + \Bigg\{ h\sum_{n=1}^{s}\sum_{l=-N}^{-1}\widetilde{\varphi}_0^{\mathrm{T}}[\widetilde{M}_A^{\mathrm{T}}(n,0)+\widetilde{M}_B^{\mathrm{T}}(n,N)]\widetilde{M}_B^{\mathrm{T}}(n,l+N)\widetilde{\psi}_l + \widetilde{\varphi}_0^{\mathrm{T}}\Bigg[(\beta+\gamma+h)I \\
& + h\sum_{n=1}^{s}[\widetilde{M}_A^{\mathrm{T}}(n,0)+\widetilde{M}_B^{\mathrm{T}}(n,N)][\widetilde{M}_A(n,0)+\widetilde{M}_B(n,N)]\Bigg]\widetilde{\psi}_0\Bigg\}.
\end{aligned}
\tag{39}
$$

Now we consider the quadratic form ${}^{h}\widetilde{\mathfrak{P}}^{\beta,\gamma}_{\alpha}(\widetilde{\varphi},\widetilde{\varphi})$ with some particular $\widetilde{\varphi}_0$, namely

$$
\widetilde{\varphi}_0 = -h[{}^{h}\mathscr{D}^{\beta,\gamma}]^{-1}\sum_{n=1}^{s}\sum_{l=-N}^{-1}(\widetilde{M}_A^{\mathrm{T}}(n,0)+\widetilde{M}_B^{\mathrm{T}}(n,N))\widetilde{M}_B(n,l+N)\widetilde{\varphi}_l,
\tag{40}
$$

where ${}^{h}\mathscr{D}^{\beta,\gamma}$ defined in (31). For $\widetilde{\varphi}_0$ defined by (40) the two last terms (within the braces) in (39) vanish and we have

$$
\begin{aligned}
{}^{h}\widetilde{\mathfrak{P}}^{\beta,\gamma}_{\alpha}(\widetilde{\varphi},\widetilde{\varphi}) = {}& \alpha h\sum_{l=-N}^{-1}\widetilde{\varphi}_l^{\mathrm{T}}\widetilde{\varphi}_l + h\sum_{n=1}^{s}\sum_{l=-N}^{-1}\sum_{m=-N}^{-1}\widetilde{\varphi}_l^{\mathrm{T}}\widetilde{M}_B^{\mathrm{T}}(n,l+N)\widetilde{M}_B(n,m+N)\widetilde{\varphi}_m \\
& - h^2\sum_{n=1}^{s}\sum_{k=1}^{s}\sum_{l=-N}^{-1}\sum_{m=-N}^{-1}\widetilde{\varphi}_l^{\mathrm{T}}\widetilde{M}_B^{\mathrm{T}}(n,l+N)(\widetilde{M}_A(n,0)+\widetilde{M}_B(n,N))[\mathscr{D}^h]^{-1} \\
& \times(\widetilde{M}_A^{\mathrm{T}}(k,0)+\widetilde{M}_B^{\mathrm{T}}(k,N))\widetilde{M}_B(k,m+N)\widetilde{\varphi}_m.
\end{aligned}
$$

The expression for ${}^{h}\widetilde{\mathfrak{P}}^{\beta,\gamma}_{\alpha}(\widetilde{\varphi},\widetilde{\varphi})$ can be written in the form

$$
{}^{h}\widetilde{\mathfrak{P}}^{\beta,\gamma}_{\alpha}(\widetilde{\varphi},\widetilde{\varphi}) = \alpha(\widetilde{\varphi},\widetilde{\varphi}) + ({}^{h}\mathscr{K}^{\beta,\gamma}_{lm}\widetilde{\varphi},\widetilde{\varphi}),
\tag{41}
$$

where

$$
\begin{aligned}
{}^{h}\mathscr{K}^{\beta,\gamma}_{lm} = {}& \sum_{n=1}^{s}\widetilde{M}_B^{\mathrm{T}}(n,l+N)\widetilde{M}_B(n,m+N) \\
& - h\sum_{n=1}^{s}\sum_{k=1}^{s}\widetilde{M}_B^{\mathrm{T}}(n,l+N)(\widetilde{M}_A(n,0)+\widetilde{M}_B(n,N)) \\
& \times[{}^{h}\mathscr{D}^{\beta,\gamma}]^{-1}(\widetilde{M}_A^{\mathrm{T}}(k,0)+\widetilde{M}_B^{\mathrm{T}}(k,N))\widetilde{M}_B(k,m+N).
\end{aligned}
\tag{42}
$$

This is the ‘discrete kernel’ in Theorem 4.1.

Theorem 4.2. *The ‘discrete kernel’* ${}^h\mathscr{K}_{lm}^{\beta,\gamma} \in \mathbb{R}^{n\times n}$ *in Theorem* 4.1 *is symmetric and positive definite* (${}^h\mathscr{K}_{lm}^{\beta,\gamma} = {}^h\mathscr{K}_{ml}^{\beta,\gamma}$ *and* $\sum\sum {}^h\mathscr{K}_{lm}^{\beta,\gamma}\widetilde{\varphi}_l\widetilde{\varphi}_m > 0$ *if* $\{\widetilde{\varphi}_l\} \neq 0$) *on* $\mathscr{F}^h$.

Proof. Using Lemma 4.1 and taking into account (41), Theorem 4.2 is established. □

Theorems 4.1 and 4.2 are valid for arbitrary s. Earlier in our discussion (see Section 2) we consider possible choices of s, which correspond to different ways of discretization of (2). It is convenient to choose $s = K$ to keep the order in the discretization of the DDEs, even if we have $\mathcal{O}(h)$ error in the quadrature in (7).

5. A discrete iterative technique

To solve the “data assimilation problem” numerically we consider the iterative process associated with (24)

$$\frac{\widetilde{y}_{n+1}^{[j]} - \widetilde{y}_n^{[j]}}{h} - A_n\widetilde{y}_n^{[j]} - B_n\widetilde{y}_{n-N}^{[j]} = f_n \quad n = 0, 1, \ldots, K-1, \tag{43a}$$

$$\widetilde{y}_n^{[j]} = \widetilde{\varphi}_n^{[j]}, \quad n = -N, \ldots, 0, \tag{43b}$$

$$-\frac{\widetilde{x}_n^{\mathrm{T}[j]} - \widetilde{x}_{n-1}^{\mathrm{T}[j]}}{h} - \widetilde{x}_n^{\mathrm{T}[j]}A_n - \widetilde{x}_{n+N}^{\mathrm{T}[j]}B_{n+N} = h[\widetilde{y}_n^{[j]}(\widetilde{\varphi}_n) - \widehat{y}_n]^{\mathrm{T}}, \tag{43c}$$

$$\widetilde{x}_n^{\mathrm{T}[j]} = 0, \quad n = K, \ldots, K+N, \tag{43d}$$

$$\widetilde{\varphi}_n^{[j+1]} = \widetilde{\varphi}_n^{[j]} + \delta_j(\alpha(\widetilde{\varphi}_n^{[j]} - \widehat{\varphi}_n) + B_{n+N}^{\mathrm{T}}\widetilde{x}_{n+N}^{[j]}), \quad n = -N, \ldots, -1, \tag{43e}$$

$$\widetilde{\varphi}_0^{[j+1]} = \widetilde{\varphi}_0^{[j]} + \delta'_j\{(\beta+\gamma+h)\widetilde{\varphi}_0^{[j]} + (I + hA_0)^{\mathrm{T}}\widetilde{x}_0^{[j]} - \beta\widehat{\varphi}_0 - (\gamma+h)\widehat{y}_0\}, \tag{43f}$$

to determine successive approximations to $\widetilde{y}$, $\widetilde{x}$ and $\widetilde{\varphi} \in \mathscr{F}^h$. The function $\widetilde{\varphi}$ obtained by the iteration process (43) provides the minimum of the functional ${}^h\widetilde{S}_\alpha^{\beta,\gamma}(\widetilde{\varphi})$. Here, $\{\delta_j\}$ and $\{\delta'_j\}$ are appropriately chosen scalars, j is an iteration index and we use the notation $\widetilde{y}_n^{[j]}$, $\widetilde{x}_n^{\mathrm{T}[j]}$ to emphasize that these are the solutions obtained by some iterative method.

We shall establish the convergence of the iterative process (43) by studying the iteration

$$\frac{\widetilde{\varphi}_n^{[j+1]} - \widetilde{\varphi}_n^{[j]}}{\delta_j} = \mathfrak{g}_n - \left(\alpha\widetilde{\varphi}_n^{[j]} + \sum_{l=-N}^{-1} {}^h\mathscr{K}_{ln}^{\beta,\gamma}\widetilde{\varphi}_l^{[j]}\right), \quad n = \{-N, \ldots, -2, -1\}, \tag{44}$$

in which j is the iteration index and we use the notation $\mathfrak{g}_n = {}^h\mathfrak{g}_\alpha^{\beta,\gamma}(n)$.

This iteration is based upon the summation equation (30). In (44), ${}^h\mathscr{K}_{ln}^{\beta,\gamma}$ has been shown to be symmetric and positive-definite; the corresponding discrete integral operator on Euclidean space with the norm $\|\psi\|_2 = (\sum_{l=-N}^{0}\psi_l^2)^{1/2}$ is bounded, self-adjoint, and positive-definite. We state the following result.

Lemma 5.1. *The iteration* (44) *is equivalent to the iteration* (43); *for a given* $\widetilde{\varphi}^{[0]}$, *the two sequences* $\{\widetilde{\varphi}^{[j]}\}$ *are identical.*

Proof. From (43e), the functions defined by the iteration (43) satisfy the relation

$$\frac{\widetilde{\varphi}_n^{[j+1]} - \widetilde{\varphi}_n^{[j]}}{\delta_j} = \alpha(\widetilde{\varphi}_n^{[j]} - \widehat{\varphi}_n) + [B_{n+N}]^{\mathrm{T}} x_{n+N}^{[j]}, \quad \text{for } n = \{-N, \ldots, -2, -1\}$$

and we have shown in Section 4.1 that $\alpha(\widetilde{\varphi}_n^{[j]} - \widehat{\varphi}_n) + [B_{n+N}]^{\mathrm{T}} x_{n+N}^{[j]} = \alpha\widetilde{\varphi}_n^{[j]} + \sum_{l=-N}^{-1} {}^h\mathscr{K}_{ln}^{\beta,\gamma}\widetilde{\varphi}_l^{[j]} - \mathfrak{g}_n$, so the result is immediate. □

Theorem 5.1 (*Convergence*). *Suppose* $\rho({}^h\mathscr{K}^{\beta,\gamma})$ *is the spectral radius of the matrix-operator* ${}^h\mathscr{K}^{\beta,\gamma}$ *on* $L_2^h[-\tau, 0]$ *defined by the 'discrete kernel'* ${}^h\mathscr{K}_{ln}^{\beta,\gamma}$. *Then, a sufficient condition for the iteration* (43) *to converge in the mean-square norm is*

$$\delta_j \leqslant \frac{2}{\max(\alpha, \rho({}^h\mathscr{K}^{\beta,\gamma}))}, \quad \textit{for all } j. \tag{45}$$

Remark 5.1. All norms on finite-dimensional Euclidean space are equivalent, so the convergence holds in any norms.

Proof. We shall write ${}^h\mathfrak{L}_\alpha^{\beta,\gamma}\widetilde{\varphi}_n = \alpha\widetilde{\varphi}_n + \sum_{l=-N}^{-1} {}^h\mathscr{K}_{ln}^{\beta,\gamma}\widetilde{\varphi}_l$ and the matrix-operator ${}^h\mathfrak{L}_\alpha^{\beta,\gamma}$ on Euclidean space with the norm $\|\cdot\|_2$ inherits self-adjointness and (with $\alpha > 0$) positive-definiteness from the corresponding properties of the matrix-operator ${}^h\mathscr{K}^{\beta,\gamma}$. For a sequence $\{\delta_j\}$ with $\delta_j > 0$ for all j, we can write the iteration process (44) in the form

$$\frac{\widetilde{\varphi}_n^{[j+1]} - \widetilde{\varphi}_n^{[j]}}{\delta_j} = \mathfrak{g}_n - {}^h\mathfrak{L}_\alpha^{\beta,\gamma}\widetilde{\varphi}_n^{[j]}. \tag{46}$$

Let $\widetilde{\varphi}_n^\star$ be the solution of the ${}^h\mathfrak{L}_\alpha^{\beta,\gamma}\widetilde{\varphi}_n^\star = \mathfrak{g}_n$ and let us define $\varepsilon^{j+1} = \widetilde{\varphi}_n^{[j+1]} - \widetilde{\varphi}_n^\star$. Then, according to (46), we have the relation $\varepsilon^{j+1} = (I - \delta_j {}^h\mathfrak{L}_\alpha^{\beta,\gamma})\varepsilon^j$, and

$$\varepsilon^{j+1} = \prod_{i=0}^{j} (I - \delta_i {}^h\mathfrak{L}_\alpha^{\beta,\gamma})\varepsilon^0. \tag{47}$$

The iteration (46) converges in the mean-square norm if $\|\varepsilon^j\|_2 \to 0$ as $j \to \infty$. From (47) we have

$$\|\varepsilon^{j+1}\|_2 \leqslant \left\| \prod_{i=0}^{j} (I - \delta_i {}^h\mathfrak{L}_\alpha^{\beta,\gamma}) \right\|_2 \|\varepsilon^0\|_2 \leqslant \prod_{i=0}^{j} \left\| (I - \delta_i {}^h\mathfrak{L}_\alpha^{\beta,\gamma}) \right\|_2 \|\varepsilon^0\|_2.$$

Thus, a sufficient condition for convergence of this iteration is

$$\|I - \delta_j {}^h\mathfrak{L}_\alpha^{\beta,\gamma}\|_2 \leqslant \vartheta < 1, \quad \text{for all } j. \tag{48}$$

Given the properties of ${}^h\mathfrak{L}_\alpha^{\beta,\gamma}$ on chosen space, we have $\|{}^h\mathfrak{L}_\alpha^{\beta,\gamma}\|_2 = \max_r \kappa_r$ (the spectral radius $\rho({}^h\mathfrak{L}_\alpha^{\beta,\gamma})$), where $\{\kappa_r\}_{r\geqslant 0}$ are the positive eigenvalues of ${}^h\mathfrak{L}_\alpha^{\beta,\gamma}$. Indeed, $\kappa_r = \alpha + \varkappa_r$, where $\{\varkappa_r\}_{r\geqslant 0}$ are the positive eigenvalues of ${}^hK^{\beta,\gamma}$. Then condition (48) becomes $\max_r |1 - \delta_j\alpha - \delta_j\varkappa_r| < 1$. We have $1 - \delta_j\alpha - \delta_j\varkappa_r \in [1 - \delta_j\alpha - \delta_j\rho({}^hK^{\beta,\gamma}), 1 - \delta_j\alpha) \subseteq (-1, 1)$ provided $1 - \delta_j\alpha - \delta_j\rho({}^hK^{\beta,\gamma}) > -1$ and Theorem 5.1 is established. □

6. Computational results

In this section, we present numerical results based upon iterative methods for the linear case (43). We start by applying the results obtained in the above section to the simplest example: the scalar linear DDE with variable coefficients and zero right-hand side,

$$\frac{\mathrm{d}y(t)}{\mathrm{d}t} - a(t)y(t) - b(t)y(t-\tau) = 0, \quad t \in [0,T], \quad y(t) = \varphi(t), \quad t \in [-\tau, 0]. \tag{49}$$

These equations are (1) with $A(t) = a(t) \in \mathbb{R}$ and $B(t) = b(t) \in \mathbb{R}$.

The criterion we used for the termination of the iterative process (43) is the condition

$$\|\widetilde{\varphi}^{[j+1]} - \widetilde{\varphi}^{[j]}\|_2 / \|\widetilde{\varphi}^{[j]}\|_2 \leqslant \varepsilon, \tag{50}$$

where $\varepsilon = 10^{-6}$ and $\|\cdot\|_2$ is the norm

$$\|\psi\|_2 = h\left(\sum_{l=-N}^{0} \psi_l^2\right)^{1/2}. \tag{51}$$

The iteration (43) terminates when (50) is satisfies and we accept the approximation obtained $\widetilde{\varphi} \equiv \widetilde{\varphi}^{[\mathscr{N}]}$, say, when $\mathscr{N} \equiv \mathscr{N}(\alpha)$. In the presentation of the experiments, together with other information, we plot $\widetilde{\varphi}$ and compare it with "true" initial function $\widetilde{\varphi}_\star$. In all numerical experiments presented here we choose time-lag $\tau = 1$ and an "observation data" $\widehat{y}(t)$ was given on a uniform mesh.

To solve test problems we obtained "pseudo-observation" data by the following procedure: we found the solution of $y(\widetilde{\varphi}_\star; t)$ of the original DDE (49) with initial function $\widetilde{\varphi}_\star$ numerically and treated this solution as the "observation data" $\widehat{y}(t)$.

6.1. *A solution with minimum norm*

In our first set of experiments, we consider the case when $\widehat{\varphi}(t) \equiv 0$. This is the case where we are seeking the solution with minimum norm in $L_2^h[-\tau, 0]$.

6.1.1. *Experiment 1*

We start with the constant coefficient case and set $a(t) = -1$ and $b(t) = -1$. We solve the problem on the interval [0,2] ($T = 2\tau$). In Experiment 1, with the "true" initial function $\widetilde{\varphi}_\star(t) = 2(0.5 + t)^3$, where $t \in [-1, 0]$, we start the iterative method (43) with initial guess $\widetilde{\varphi}^{[0]} = 0$. In the numerical experiments described below we took 64 points in $[-1, 0]$.

First, we investigate how the convergence of the iteration method depends on the regularization parameter α. The number of iterations and the cpu time needed to obtain the required accuracy $\varepsilon = 10^{-6}$ are given in the Table 1 for different α. The figures for cpu time are unreliable because the computer is not a dedicated computer, but this give some indication of the time. Introducing a regularization parameter α leads to a solution $\widetilde{\varphi} \equiv \widetilde{\varphi}^{[\mathscr{N}]}(\alpha)$, which differs from the solution $\widetilde{\varphi}_\star$. We denote the relative error by the expression

$$\mathscr{R} \equiv \frac{\|\widetilde{\varphi}^{[\mathscr{N}]} - \widetilde{\varphi}_\star\|_2}{\|\widetilde{\varphi}_\star\|_2},$$

Table 1
The number of iterations $\mathcal{N}$ and relative error $\mathcal{R}$ versus the regularization parameters α

α	1	0.5	0.2	0.1	0.01	0.001	0.0001	0
The number of iterations $\mathcal{N}$	432	690	1302	2068	9746	26205	36226	38176
cpu time min:sec	0:00.5	0:00.8	0:01	0:02	0:05	0:11	0:27	0:31
The relative error $\mathcal{R}$	0.894	0.851	0.751	0.646	0.294	0.088	0.043	0.038

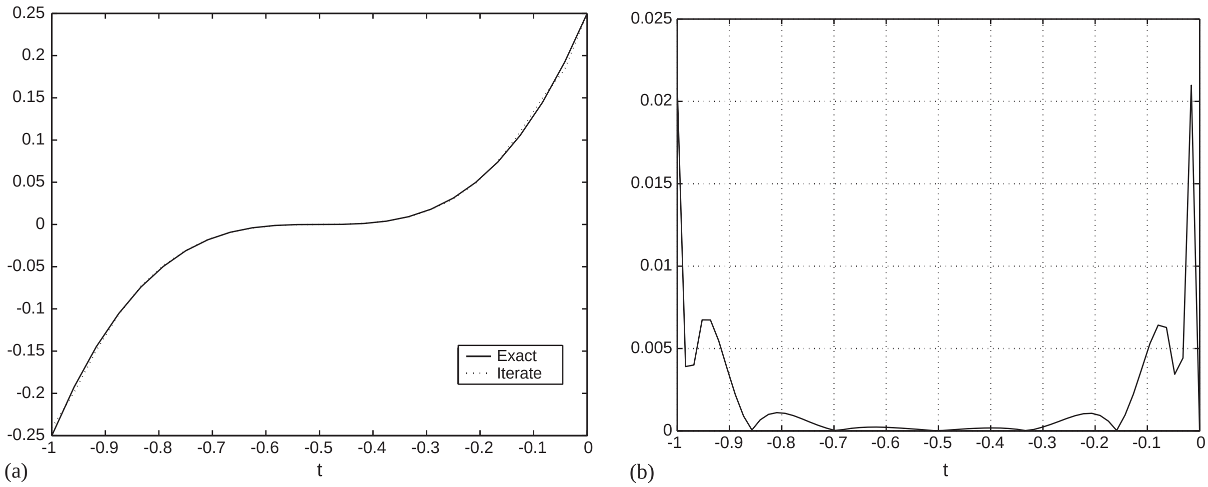

Fig. 1. An experiment with the parameter $\alpha = 0$: (a) The exact function $\widetilde{\varphi}_\star(t)$ (solid line) and the iterated function $\widetilde{\varphi}^{[\mathcal{N}]}(t)$, $\mathcal{N} = 38176$; (b) The difference curve $|\widetilde{\varphi}_\star(t) - \widetilde{\varphi}^{[\mathcal{N}]}(t)|$.

where $\widetilde{\varphi}^{[\mathcal{N}]}$ is the iterated solution found by (43) and $\|\cdot\|$ is the norm defined in (51). Table 1 gives the value of relative error for different α.

We see from Table 1, that the introduction of a regularization parameter α speeds up the convergence of the iterative method. This is one of the advantages of introducing the regularizer. The disadvantage, as we can see in Table 1, is that the parameter α leads to an error in the identified solution (Fig. 1). (In the table displayed the error decreases with α.)

6.1.2. *Experiment 2*

The qualitative behaviour of $\widetilde{\varphi}^{[\mathcal{N}]}(\alpha)$ with respect to the regularization parameter α is typical of that seen with other problems (having differing $\varphi(t)$ and differing $\widetilde{\varphi}^{[0]}$). To illustrate the last remark let us consider the second experiment with the "true" initial function $\widetilde{\varphi}_\star(t) = 10\exp(1/(t(1-t)))$. The number of points on the initial interval is 64.

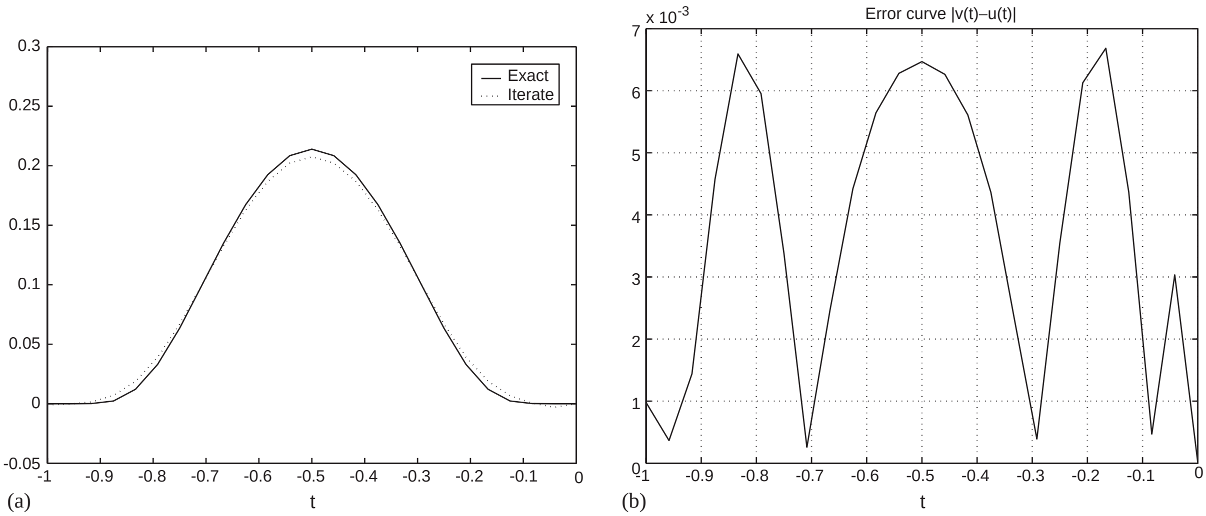

Fig. 2. An experiment with the parameter $\alpha = 0.001$: (a) The exact function $\widetilde{\varphi}_{\star}(t)$ (solid line) and the iterated function $\widetilde{\varphi}^{[\mathscr{N}]}(t)$; (b) The difference curve $|\widetilde{\varphi}_{\star}(t) - \widetilde{\varphi}^{[\mathscr{N}]}(t)|$, $\mathscr{N} = 16434$.

Table 2
The number of iterations versus the regularization parameters α: experiment 2

α	1	0.5	0.2	0.1	0.01	0.001	0.0001	0
The number of iterations $\mathscr{N}$	327	550	1172	2066	8127	16434	19058	19416
The relative error $\mathscr{R}$	0.862	0.776	0.642	0.543	0.207	0.036	0.012	0.01

The results of this experiment are presented in Fig. 2 and a summary in Table 2. The relative error decreases when the parameter α decreases.

6.1.3. Experiment 3

In the next series of experiments, we consider a variable coefficient case. In Experiment 3 the "exact" initial function is $\widetilde{\varphi}_{*}(t) = 2(0.5 + t)^3$. The parameters are follows: $\alpha = 0$, $\beta = 0$, $\gamma = 1$. In the experiment presented in Fig. 3 the coefficients of the Eq. (49) are

$$a(t) = -1 + \sin(\pi t), \quad b(t) = -2t, \quad \text{where } t \in [0, 4]. \tag{52}$$

6.2. A rôle for the function $\widehat{\varphi}$

In this section we discuss the rôle for the function $\widehat{\varphi}(t)$. We shall present results, which may have a practical significance.

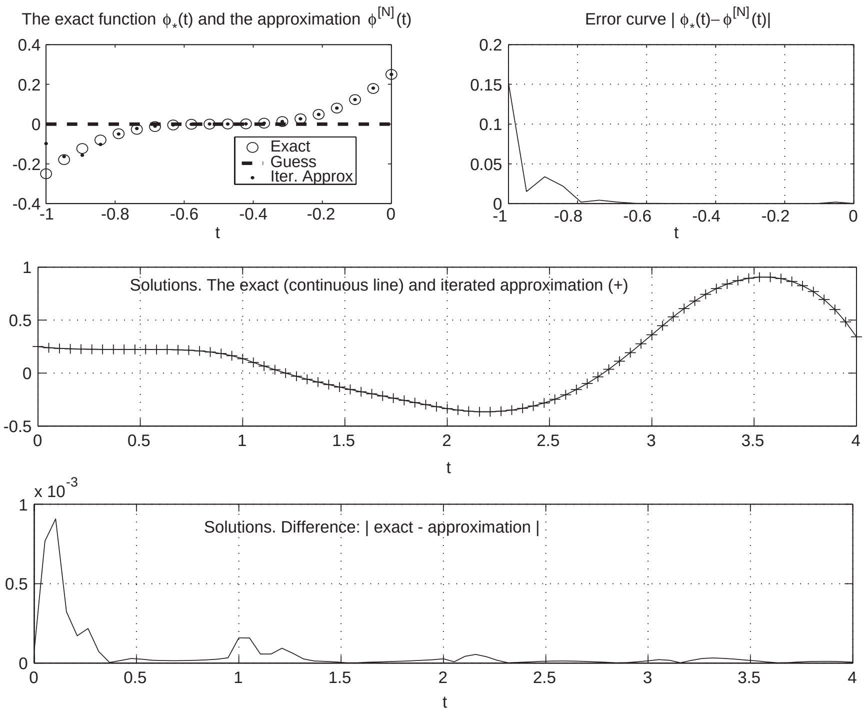

Fig. 3. An experiment with $a(t)$ and $b(t)$ defined by (52): number of iterations $\mathcal{N} = 139374$, cpu time: 0 min 08.99 s, number of initial points 20, accuracy 10^{-6}, parameters $\alpha = 0$, $\beta = 0$, $\gamma = 1$, relative error $\mathcal{R} = 0.323$, functional ${}^{h}\widetilde{S}_{\alpha}^{\beta,\gamma}(\varphi)$: starting value 0.038, final value: 4.77×10^{-9}.

In the next experiment suppose that we have some information about the initial function (its general form, some coefficients, etc.) and want to improve this information. For example, we know the general form of the initial function, but we need to correct some coefficients.

As an example, we consider the function

$$\widetilde{\varphi}(t) = \sigma_1 \exp\left(\frac{\sigma_2}{t(t+1)}\right),$$

here, the structure is assumed but we suppose σ_1 and σ_2 unknown. Observe that we do not estimate σ_1, σ_2 but compute the mesh values of an approximation $\widetilde{\varphi}$ to $\widetilde{\varphi}_\star$.

For the "true" initial function we take the following coefficients: $\sigma_1 = 500$, $\sigma_2 = 1.8$ and for the function $\widehat{\varphi}$, $\sigma_1 = 10$, $\sigma_2 = 1$. The number of initial points is 50. In the Table 3 we give a summary of an experiment. The exact initial function, the function $\widehat{\varphi}$ and the iterated solution, which we accept as on approximation to $\widetilde{\varphi}$, are shown in the Fig. 4.

As we see from this experiment the behaviour of the accepted iterate function depends on the regularization parameter α. When $\alpha \approx 1$ the approximate solution is relatively close to the function $\widehat{\varphi}$; when $\alpha \to 0$ the accepted function becomes closer to the "true" initial function.

It can be shown, that in the case when the integral equation of the first kind ($\alpha = 0$) has a unique solution, the resulting approximate solution is independent of the function $\widehat{\varphi}$. When there is not a unique solution, the choice of $\widehat{\varphi}$ influences $\widetilde{\varphi}_\star$ as $\alpha \to 0$.

Table 3
A summary of the experiments

The parameter α	1	0.1	0.01	0.001
The number of iterations	372	2415	10499	21598
CPU time (min:sec)	0:02	0:11	0:50	1:54
The relative error	0.471	0.365	0.006	0.002

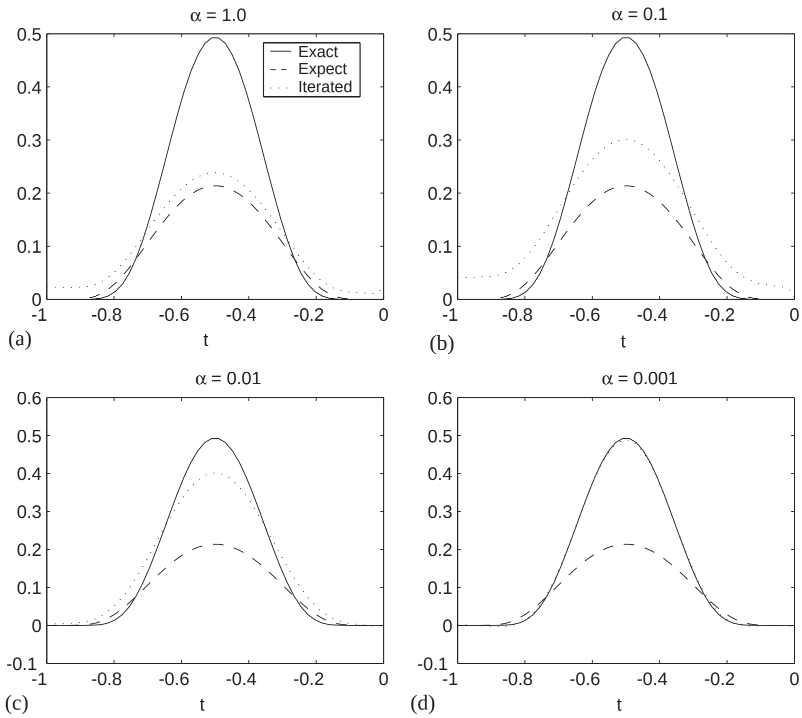

Fig. 4. The rôle of $\widehat{\varphi}$ for different α: experiment 4.

6.3. A jump at the initial point

Another problem, which can arises for DDE is a jump in the initial function at the initial point t_0 (in our case $t_0 = 0$). In Section 4, we write the equivalent formulation for the first variation of the functional (2) and obtain two equations for the initial function (24e) and (24f). Therefore, it is easy to see that we can extend the identification problem to the case where the initial function has a jump. Let us consider the numerical experiment with the "true" initial function in the form

$$\widetilde{\varphi}_\star(t) = \begin{cases} \sqrt{1+t}, & t \in [-1, 0), \\ 2, & t = 0. \end{cases} \tag{53}$$

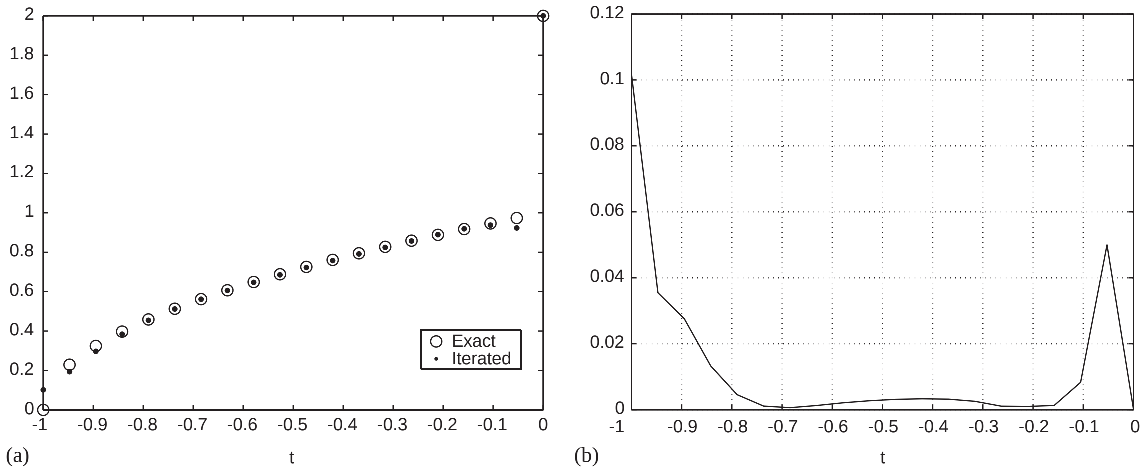

Fig. 5. An experiment with a jump at the initial point when the exact initial function is (53): (a) The exact function $\widetilde{\varphi}_\star(t)$ (solid line) and the iterated function $\widetilde{\varphi}^{[\mathcal{N}]}(t)$, $\mathcal{N} = 38420$; (b) The difference curve $|\widetilde{\varphi}_\star(t) - \widetilde{\varphi}^{[\mathcal{N}]}(t)|$.

The parameters in this experiment are taken to be $\alpha = 0$, $\beta = 0$, $\gamma = 1$, the coefficients are $a(t) = -1$ and $b(t) = -1$. The number of points on the initial interval is 20 and $T = 4$. The results are shown in Fig. 5.

From the above figures we see, that results obtained for initial function with jump is similar to that obtained for a continuous initial function.

6.4. An experiment with perturbed data

In practice, data observed from physical experiments always has some noise. Therefore, to justify our approach we need some numerical experiments where a perturbation is added to the "observation data". To investigate the behaviour of the iterative method we add to our "observation data" $\widehat{y}(t)$ a noise $\sigma\eta(t_i)$, where $\eta(t_i) \in N[0, 1]$, $t_i = ih$. Then we solve the identification problem of finding the initial function with "new observation data" $\widehat{y}(t_i) + \sigma\eta(t_i)$. Here we use a scalar factor $\sigma \in \mathbb{R}$ to obtain a sufficiently small noise (approximately 5% of the "observation data").

One of the experiment with perturbed "observation data" is shown in Fig. 6. In this experiments the "true" initial function is $\widetilde{\varphi}_*(s) = 50 \exp 1/(s(1-s))$, where $s \in [-1, 0]$. The coefficients of Eq. (49) are $a(t) = -2t$ and $b = t$, where $t \in [0, 4]$.

Thus, we can conclude that, in the current experiment and run on for sufficiently small noise, the method allows us to recover an initial function with reasonable accuracy.

6.5. Concluding remarks

Here we considered the identification problem through the example of simple linear DDEs. The main experimental results are as follows.

If the regularization parameter α is equal to zero, the convergence rate of the method presented (the Picard iteration) is very slow and the result can be quite inaccurate. In general, we found the greatest error at the end points.

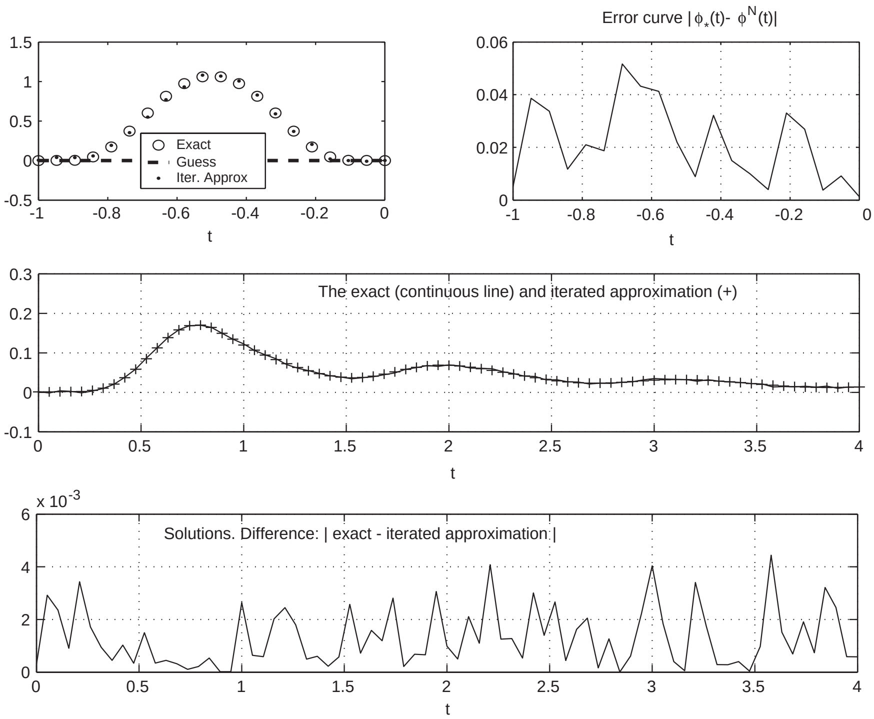

Fig. 6. An experiment with perturbed “observation data”: number of iterations $\mathscr{N} = 67264$, cpu time: 0 min 11.56 s, number of initial points 20, accuracy 10^{-6}, parameters $\alpha = 0$, $\beta = 0$, $\gamma = 1$, relative error $\mathscr{R} = 0.035$, functional ${}^h\widetilde{S}_\alpha^{\beta,\gamma}(\varphi)$: starting value 9.58×10^{-4}, final value: 4.33×10^{-7}.

The introduction of a regularization parameter α speeds up the convergence. We solve an integral equation of second kind with symmetric and positive-definite kernel. A disadvantage of introducing a regularization parameter lies in the fact that an error, which depend on α, is introduced to the solution. The error decreases with α, but, at the same time, the number of iteration increases. The dependence on β and γ is not so strong, compared with the dependence upon α. In fact, when $\alpha = 0$ and β and γ are nonnegative, we still have to solve an integral equation of the first kind.

Numerical experiments also show that the iterative method proposed can be used to solve the problem, when the initial function has a jump at the initial point. The behaviour of the algorithms in this case is similar to that we have for a continuous initial function.

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References

[1] V.I. Agoshkov, Optimal control methods in inverse problems and computational processes, J. Inverse Ill-Posed Probl. 9 (2001) 205–218.

[2] V.I. Agoshkov, G.I. Marchuk, On the solvability and numerical solution of data assimilation problems, Russian J. Numer. Anal. Math. Modelling 8 (1993) 1–16.
[3] V.I. Agoshkov, E.I. Parmuzin, V.P. Shutyaev, C. Bardos, Numerical analysis of iterative algorithms for an inverse boundary transport problem, Math. Models Methods Appl. Sci. 10 (2000) 11–29.
[4] C.T.H. Baker, G.A. Bocharov, C.A.H. Paul, Mathematical modelling of the Interleukin-2 T-cell system: a comparative study of approaches based on ordinary and delay differential equations, J. Theor. Med. 2 (1997) 117–128.
[5] C.T.H. Baker, G.A. Bocharov, C.A.H. Paul, F.A. Rihan, Modelling and analysis of time-lags in some basic patterns of cell proliferation, J. Math. Biol. 37 (1998) 341–371.
[6] C.T.H. Baker, G.A. Bocharov, C.A.H. Paul, F.A. Rihan, Computational modelling with functional differential equations: identification, selection, and sensitivity, Appl. Numer. Math. (available online 19 October 2004), in press.
[7] C.T.H. Baker, E.I. Parmuzin, A guided tour of VPF for continuous and discretized DDEs, NA Report 430, MCCM, Manchester, England, September 2003.
[8] C.T.H. Baker, E.I. Parmuzin, Identification of the initial function for a delay differential equation: part I: the continuous problem and an integral equation analysis, NA Report 431, MCCM, Manchester, England, September 2003, ISSN: 1360-1725.
[9] C.T.H. Baker, E.I. Parmuzin, Analysis via integral equations of an identification problem for delay differential equations, J. Integral Equations Appl. 16 (2004) 111–135.
[10] H.W. Engl, M. Hanke, A. Neubauer, Regularization of inverse problems, Mathematics and its Applications, vol. 375, Kluwer Academic Publishers Group, Dordrecht, 1996, ISBN 0-7923-4157-0.
[11] V.B. Kolmanovskii, L.E. Shaikhet, Control of Systems with Aftereffect, AMS, Providence, RI, 1996, ISBN 0-8218-0374-3.
[12] F.-X. Le Dimet, O. Talagrand, Variational algorithms for analysis and assimilation of meteorological observations, Tellus A 38 (1986) 97–110.
[13] G.I. Marchuk, V.B. Zalesny, A numerical technique for geophysical data assimilation problem using Pontryagin's principle and splitting-up method, Russian J. Numer. Anal. Math. Modelling 8 (1993) 311–326.
[14] E.I. Parmuzin, V.P. Shutyaev, Numerical analysis of iterative methods for solving evolution data assimilation problems, Russian J. Numer. Anal. Math. Modelling 14 (1999) 275–289.
[15] V. Shutyaev, Control operators and iterative algorithms in variational data assimilation problems, J. Inverse Ill-Posed Probl. 9 (2001) 177–188.
[16] S.M. Verduyn Lunel, Parameter identifiability of differential delay equations, Internat. J. Adapt. Control Signal Process. 15 (2001) 655–678.